Asymptotic Dynamics of Breathers in Fermi-Pasta-Ulam Chains

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We study the asymptotic dynamics of breathers in finite Fermi-Pasta-Ulam chains at zero and non-zero temperatures. While such breathers are essentially stationary and very long-lived at zero temperature, thermal fluctuations tend to lead to breather motion and more rapid decay.

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I. INTRODUCTION

Energy localization in the form of breathers has been intensely investigated over the past several years [1]. These highly localized long-lived excitations in translationally invariant nonlinear arrays are of great interest because they provide a mechanism for energy storage that does not rely on defects. Indeed, the fact that these excitations are often mobile (which they would in general not be if the localization were defect-induced) makes them particularly interesting in the context of efficient transport of vibrational energy [2].

Exact breather excitations, that is, breathers that persist forever, can be confirmed analytically and constructed numerically for certain nonlinear infinite arrays of interacting masses, among them nonlinear arrays with no local potentials and interactions between neighboring sites that vary as $(x_i - x_j)^n$ with $n \to \infty$ [3]. The x's denote displacements of the masses at sites i and j. When the interactions are not precisely of this form, or when the array is finite, or when other excitations (for example, phonons or other localized excitations) are present in the system, it is no longer possible to prove that there are exact breather solutions. Nevertheless, it is possible to explore the problem numerically. In particular, in this paper we study the asymptotic dynamics of localized excitations in the one-dimensional Fermi-Pasta-Ulam (FPU) β-model at zero temperature and during thermal relaxation. We corroborate that long-wavelength thermal excitations have a profound effect on breather stability. Since thermal fluctuations are inevitable in any real system, zero-temperature results must be applied with appropriate caution. These results extend our earlier work to much longer time regimes [4, 5], and agree with and complement those of Piazza et al. [6]. The conditions for breather stationarity and longevity are thereby further clarified. We present our numerical results in Secs. II and III, and end with a brief summary in Sec. IV.

II. BREATHERS AT ZERO TEMPERATURE

The Hamiltonian for the FPU β-model is

$$H = \sum_{i=1}^{N} \frac{\dot{x}_i^2}{2} + \frac{k}{2}\sum_{i=1}^{N}(x_i - x_{i-1})^2 + \frac{k'}{4}\sum_{i=1}^{N}(x_i - x_{i-1})^4, \tag{1}$$

where N is the number of sites, and k and k' are the harmonic and anharmonic force constants, respectively. We set $k = k' = 0.5$ throughout. The equations of motion with free-end boundary conditions are integrated using a fourth order Runge-Kutta method with time interval $\Delta t = 5 \times 10^{-4}$ (further reduction leads to no significant improvement). The total energy of the array is the sum over individual symmetrized site energies $E_i(t)$ [4]. A zero temperature environment with the least disturbance to the dynamics in the chain is achieved by connecting only the ends of the chain to such an environment via a dissipation term. This is accomplished by adding a term of the form $-\gamma\dot{x}_i$ to the equations of motion for sites $i = 1$ and $i = N$ [4, 6].

Since we do not *a priori* know the form of the longest-lived localized excitation, we initially create an excitation of the "odd parity" breather configuration with amplitudes $(0, \cdots, 0, -A/2, A, -A/2, 0, \cdots, 0)$, and zero velocity at each site. The frequency of the resulting oscillatory motion increases with increasing A, which must be chosen so

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that this frequency is above the phonon band edge at $\omega = \sqrt{2}$. This excitation is not an exact stationary solution of the equations of motion, so it typically sheds some energy while re-accommodating amplitudes and frequencies, and settles into an excitation that is very long-lived. The discarded energy appears in the form of phonons that travel away from the localized excitation and dissipate quickly, in a time τ_m, across the ends of the chain. The balance of the energy remains localized, most of it (98% for $A = 0.5$) on the three initially excited sites, and decays exponentially with an extremely long characteristic time τ.

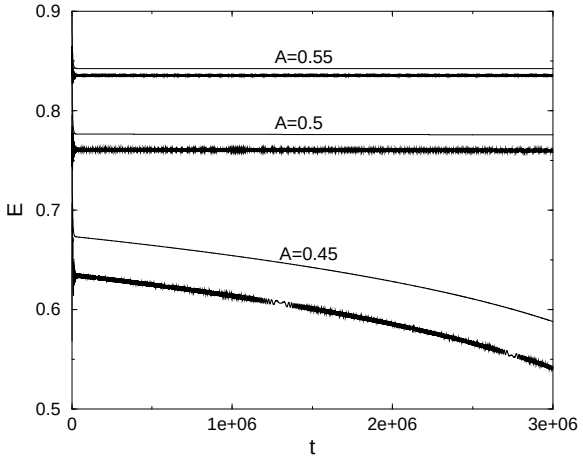

FIG. 1: Decay of the normalized energy $E(t)$ for three different values of the initial amplitude A for chains of $N = 31$ sites connected at the ends to a zero-temperature bath. The dissipation parameter $\gamma = 1$. The thin lines represent the total energy remaining in the chain, and the bold lines the portion of the remaining energy that is localized on the three initially excited sites.

To extract exponents and characteristic times, it is crucial to have data that covers both time scales, and to normalize the data in such a way that one behavior does not mask or distort the other [7]. We introduce the *normalized energy* $E(t)$ and the *modified normalized energy* $E_m(t)$:

$$E(t) \equiv \frac{\sum_{i=1}^{N} E_i(t)}{\sum_{i=1}^{N} E_i(0)}, \qquad E_m(t) \equiv \frac{\sum_{i=1}^{N} E_i(t)}{\sum_{i=1}^{N} E_i(\tau_m)}. \tag{2}$$

The denominator in the first contains the initial energies, and in the second the energies after the discarded phonons have dissipated (but before the remaining localized excitation has decayed appreciably). In our illustrations we take $\tau_m = 40,000$.

In Fig. 1 we show typical results for the normalized energy for three excitation amplitudes over more than six decades of time. The modified normalized energy shows essentially the same behavior. If the decay of the long-lived excitation is exponential, we expect $[-\log E(t)]$ and $[-\log E_m(t)]$ vs t to be straight lines over the appropriate long time intervals. In Fig. 2 we clearly see this behavior, which extends over the entire time interval for the higher (but not the lower) amplitude excitation. The slope for the $A = 0.5$ curve leads to a decay time of $\tau = 5.32 \times 10^9$, a number reported here merely to stress its enormous magnitude. The frequency of the localized breather increases with increasing amplitude and hence is more separated from the phonon band for larger A, leading to a slower decay of more energetic breathers. As the breather loses its energy, its frequency decreases, and eventually as it approaches the phonon band edge the decay becomes more rapid. This behavior is evident in the $A = 0.45$ curve in Fig. 2. We also find that longer chains exhibit a longer decay time: residual amplitude of the breather at sites far from its center decreases rapidly with increasing distance and thus the chain end sites have less energy to dissipate.

Figure 3 confirms the exponential behavior of the breather decay [6, 7]. For two initial amplitudes, the figure shows $[\log(-\log E_m(t))]$ vs $\log t$, which yields a straight line of slope β if the decay is of the form $E_m(t) \propto e^{(-t/\tau)^\beta}$. The inset shows the values of the slopes as a function of time. For $A = 0.5$ pure exponential behavior $\beta = 1$ is confirmed throughout the time range presented. The deviation from pure exponential decay for the lower amplitude breather is evident.

A breather of a given amplitude has a well-defined characteristic frequency. In Fig. 4 we show this frequency in relation to the phonon band edge as a function of time for the cases discussed above. For 31-site chains, the frequency

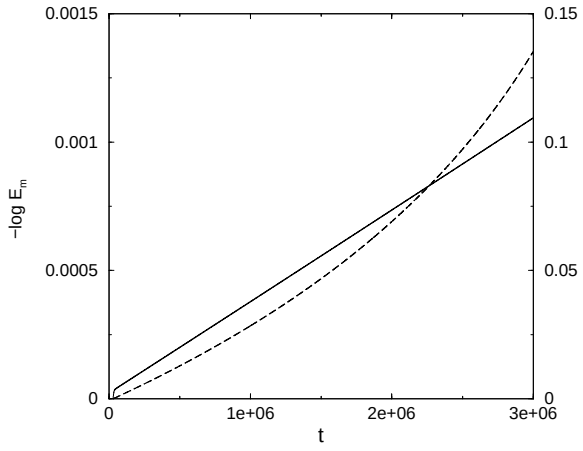

FIG. 2: $[-\log E_m(t)]$ vs t for two initial amplitudes, $A = 0.5$ (solid curve, left scale) and $A = 0.45$ (dashed curve, right scale) for a chain of 31 sites.

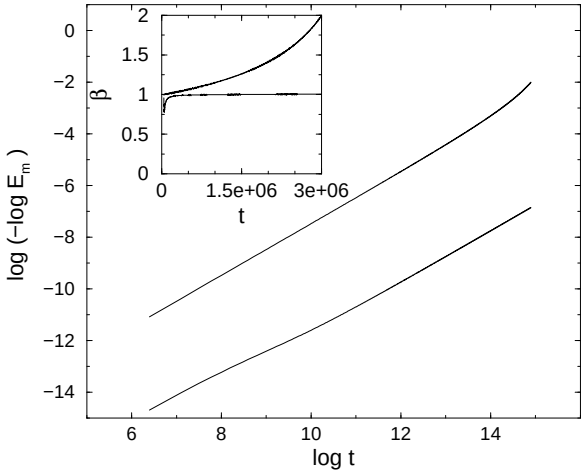

FIG. 3: $[\log(-\log E_m(t))]$ vs $\log t$ for two initial amplitudes, $A = 0.5$ (lower curve) and $A = 0.45$ (upper curve) for a chain of 31 sites. The inset shows the associated slopes. Lower curve: $A = 0.5$; upper curve: $A = 0.45$.

of the breather of initial amplitude $A = 0.5$ decreases very little over the entire simulation, while that of initial amplitude $A = 0.45$ decreases more markedly. Consistent with the fact that the breather does not disappear entirely in the time range shown, its frequency never reaches the phonon band edge. If the initial amplitude of the excitation were even smaller, or the simulation time much longer, or the chain shorter, the breather would eventually disappear. This last case is illustrated in Fig. 4. The disappearance of the breather coincides with its frequency reaching the band edge. The inset shows L, the ratio of the energy on the five sites around the breather to the total energy. This parameter is of order unity when most of the energy is localized on a small number of sites.

III. BREATHERS AT FINITE TEMPERATURES

The situation is less certain when a localized excitation evolves in a thermal environment. Other excitations in the medium perturb the breather, and its eventual fate varies from one realization to another. To illustrate the complexity of the situation, we present two scenarios.

We begin with a chain that is initially in thermal equilibrium at a nonzero temperature $T \neq 0$ [4]. At time $t = 0$,

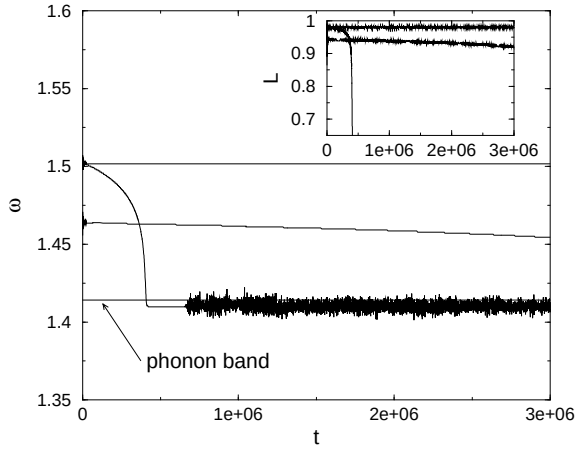

FIG. 4: Breather frequency as a function of time. Upper curve: $A = 0.5$, $N = 31$. Middle curve: $A = 0.45$, $N = 31$. Lower curve: $A = 0.5$, $N = 21$. Inset: associated localization parameters in the same order.

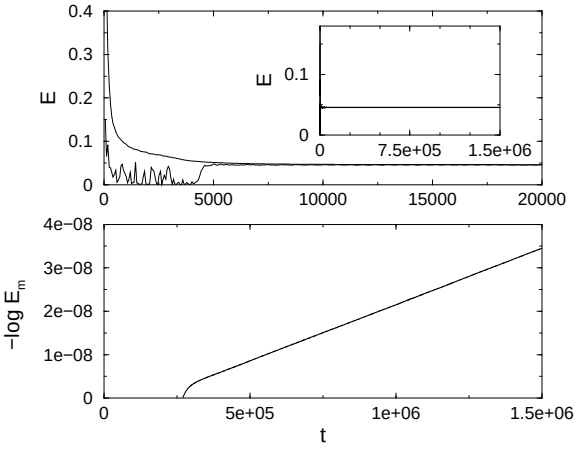

FIG. 5: Upper panel: the smooth curve is the normalized energy as a function of time for a chain of 30 sites initially thermalized at $T = 0.5$ and connected through its ends to a zero-temperature heat bath ($\gamma = 0.1$). The initially jagged curve is the normalized energy on sites 13, 14, 15, and 16. The inset shows the temporal evolution of the energy on these four sites over a longer time scale. Lower panel: $[-\log E_m(t)]$ vs t for the same chain.

the end sites of the thermalized chain are connected to a zero temperature bath via a purely dissipative term [4, 6, 8]. We follow the thermal relaxation of the chain and, in particular, the dynamics of breathers that may spontaneously appear during relaxation if the initial temperature is sufficiently high.

Figure 5 shows the evolution of the total energy in a chain of 30 sites initially thermalized at temperature $T = 0.5$. The figure also shows the energy in only the four sites $i = 13, 14, 15, 16$. After a relatively short time (5000 time units in this particular realization) almost all of the energy settles in these sites and remains there. The excitation around the four sites turns out to be an "even parity" breather, with maximum displacements A and $-A$ alternating on sites 14 and 15, smaller but not negligible amplitudes at sites 13 and 16, and essentially no motion of the other sites. The frequency of the breather, initially $\omega = 1.633$, decreases very little for the duration of the simulation. In Fig. 5 we also present the modified normalized energy. Its decay is clearly exponential, with an enormously long time constant, $\tau = 4 \times 10^{13}$. Thus this breather, even in our relatively short chain, is essentially stationary. This decay time is much longer than that reported in the previous section, consistent with the fact that the amplitude of the breather that has emerged spontaneously is larger. The thermal relaxation process has swept the lattice clean of all other excitations, allowing the breather to survive undisturbed. This process was described in our earlier work [4, 5].

There we reported a stretched exponential rather than a purely exponential decay, a conclusion that relied on the normalized rather than the modified normalized energy [7], on a time history that was not sufficiently long, and on a statistical average over a thermal ensemble that included realizations where no breather appeared during the thermal relaxation process (and where the energy dissipation was consequently much more rapid).

In our second scenario, at $t = 0$ a breather is explicitly injected into a chain that is in thermal equilibrium at a very low temperature (too low for the spontaneous formation of breathers). The chain is then allowed to relax into a zero temperature heat bath. We find that the thermal background invariably sets the breather in motion, and causes the breather to collide with other excitations and with the chain boundaries. Collision events not only cause the breather to keep moving, but also lead to breather degradation through loss of energy upon collision [4, 5]. The resulting lifetime τ of the breather is then in general much smaller than in the first scenario. The lifetime is also much smaller than that of a breather of the same amplitude injected into a zero temperature chain. We find this behavior even when the temperature is extremely low (all the way down to $T = 10^{-7}$). As a quantitative check we have explicitly injected a breather of initial amplitude $A = 0.5$ into a chain thermalized at $T = 10^{-6}$. The system is then allowed to relax into a zero temperature bath, as before. Compared to the lifetime of the breather in the zero temperature chain, the lifetime of the breather is now much reduced, $\tau = 1.3 \times 10^6$. A similar comparison with $A = 0.55$ again leads to dramatically different lifetimes, $\tau = 1.426 \times 10^{11}$ ($T = 0$) and $\tau = 2.1 \times 10^6$ ($T = 10^{-6}$). Note that it does not much matter whether the injected breather is of even or odd parity (we inject an odd one).

Why is a breather created spontaneously during thermal relaxation more stable than one explicitly injected into a thermalized chain, even at extremely low temperatures? The answer lies in the effect of different phonons on breather dynamics [4, 5, 6]. Whereas short wavelength zone-boundary phonons contribute to spontaneous breather formation ("modulational instability"), breathers are most strongly perturbed by the longest wavelength phonons. These are also the phonons that dissipate most rapidly out of a chain with free-end boundaries into a zero-temperature bath. In the higher temperature system, when the breather is created spontaneously the long wavelength phonons have already dissipated and, as dissipation continues up the phonon spectrum, the breather is increasingly less disturbed until it reaches a spatially stationary very long-lived configuration [4]. On the other hand, if the breather is injected into a thermalized system, the breather is subject to strong disturbance by long wavelength phonons even at the very lowest temperatures until these phonons dissipate. An injected breather in the thermalized scenario is therefore a more fragile excitation than a spontaneously created breather of the same amplitude. To confirm this description we have followed the dynamics of a breather injected into a relaxing chain *after* the long wavelength phonons have decayed, and find the breather to be almost as stable as one in a zero-temperature simulation. For example, for a zero-temperature injected breather of initial amplitude $A = 0.6$ in a chain of 31 sites ($\omega = 1.65$), we find a lifetime $\tau = 3.10 \times 10^{14}$. In a chain initially thermalized at $T = 10^{-5}$ and then allowed to relax, if we wait until $t = 15,000$ before injecting the same breather we find a somewhat shortened but still very long lifetime of $\tau = 6.15 \times 10^{13}$, in any case much longer than it would be if injected at $t = 0$. We have also observed a breather in a chain whose temperature is maintained at an extremely low but nonzero value. The breather in this case is always fragile, continuing to move and lose energy until it degrades completely. The zero temperature stability of the breather is therefore a somewhat singular result.

IV. SUMMATION

Our work supports three main conclusions concerning the dynamics of breathers in FPU β-chains: 1) At zero temperature in finite chains, breather-like excitations remain stationary and localized, and their energy decays exponentially with time; 2) The decay time at zero temperature is extremely long, increasing with increasing chain length and with increasing initial breather amplitude; 3) Long wavelength thermal background sets the breather in motion, which in turn leads to a more rapid decay of the breather. The zero-temperature result is in this sense fragile.

We have confirmed that breather decay for any particular realization is exponential [6] until the breather frequency closely approaches the phonon band edge. However, since the characteristic exponential time varies considerably from one realization to another, an ensemble averaged decay may be of stretched exponential or other form.

Acknowledgments

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